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Protonium formation in arbitrary excited states

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Abstract : We carry out a full quantum mechanical calculation of the total cross sections for the rearrangement process $\bar{p} + H(1s) \rightarrow p\bar{p}(nlm) + e^-$ ein the Born approximation considering the full interaction. This treatment is applied to another first order approximation — the distorted wave approximation, which aims at an improvement over the Born approximation by incorporating the non-orthogonality effect. The protonium $(p\bar{p})$ formation corss sections in the above mentioned approximations have been presented for a wide range of incident antiproton energies and their variations with the quantum numbers have been studied. It has been observed that the cross sections have a tendency to become appreciable when the protonium atom is formed in an excited state having a moderate or high value of n as well as when the incident energy is low.

Keywords . Antiproton, hydrogen atom, protonium, arbitrary excited states.

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1. Introduction

The protonium $(p\bar{p})$ atom – an electromagnetically bound system of a proton and an antiproton – is of particular interest because of its importance in many branches of physics such as atomic, nuclear and particle physics. The traditional way of forming protonium is by stopping antiprotons in high density hydrogen. As a probe, protonium looks quite interesting for the study of nuclear force at low energy [1,2] and also for the study of the colour force between quarks [3]. Investigations in the field of excitation and ionization in antiproton atom collisions represent an important part of the experimental activity at the CERN with its low-energy antiproton ring (LEAR) facilities which has been in operation since 1983. Theoretically the formation of protonium in low energy collisions of antiprotons with protons, neutral and negatively ionised hydrogen atom has been studied by Bracci *et al* [4] using a purely classical method. The process of protonium formation at very low energy has been extensively studied by Cohen [5–7], employing the classical-trajectory Monte Carlo (CTMC) method. The CTMC method has also been used by Schultz *et al* [8] to investigate $p\bar{p}$ formation process. Recently a semiclassical approach has been presented by Sakimoto [9] for $p\bar{p}$ formation at energy less than 10 eV where the time-dependent Shrödinger equation is directly solved using a discrete-variable-representation (DVR) technique. However, in order to have a thorough understanding of the protonium formation process, a rigorous full quantum mechanical approach is highly needed. With a view to this, we in this paper, have carried out a detailed full quantum mechanical calculation of the total cross section for the formation of protonium in an arbitrary excited state (nlm) in antiproton hydrogen atom collisions. Since protonium is formed mostly in very high orbital states [5,6,10], full quantum mechanical calculation becomes very much complicated due to the presence of a large number of oscillations in the bound state wave

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functions of protonium formed in the final channel. In view of such complications, we have carried out our calculations in the framework of the first Born approximation (FBA) considering the full interaction and taking into account the complete arbitrariness of all the quantum numbers n, l and m. On using the FBA the analytical treatment becomes relatively simple without hampering the qualitative understanding of the general features of the collision process. Moreover, the proposed technique is quite straightforward and rather simple in the sense that all the cross sections can easily be obtained from a single computer code. This in turn, makes it possible to have a comparative study of the variation of the protonium formation cross section with the quantum numbers n, l and m.

It is well known that the simple FBA does not take into account the effect of the lack of orthogonality of the initial and the final state wave functions, the reason for the non-orthogonality being the different zero-order Hamiltonians for the initial and the final channels. With an aim to have an improvement over the Born approximation the above technique has been applied to another first order approximation – the distorted wave approximation (DWA) – which incorporates the non-orthogonality effect according to Bates [11] and Bassel and Gerjuoy [12].

2. Theory

We consider the following rearrangement process

$$\bar{p} + H(1s) \rightarrow p\bar{p}(nlm) + e^- \tag{1}$$

in the center of mass co-ordinate system.

In the first Born approximation, the protonium formation amplitude in atomic units, may be written as

$$g_{if}^{\mathrm{FBA}} = -\frac{2M}{2\pi(2M+1)} \times \int \exp[i(\alpha.r_2 - \beta.r_1)]\, \phi_f^*(r_1) V \phi_i(r_2)\, dr_1 dr_2, \tag{2}$$

where r_1 and r_2 are, respectively, the position vectors of the antiproton and the electron with respect to the target proton, M is the proton mass and V is the post form of interaction given by

$$V = \frac{1}{|r_1 - r_2|} - \frac{1}{r_2}. \tag{3}$$

It may be mentioned here that the question of post-prior discripancy does not arise in the present case since the hydrogen- and the protonium-atom wave functions are exact. The vectors α and β are given by

$$\alpha = -k_f - \frac{k_i}{M+1} \qquad \beta = -k_i - \frac{k_f}{2}, \tag{4}$$

where k_i and k_f are, respectively, the initial momentum vector of the antiproton relative to the center of mass of the initial system and the final momentum vector of the protonium atom relative to the electron. The initial and final bound-state wave functions corresponding to the target hydrogen atom in the ground state and the protonium atom in an arbitrary excited state (nlm), respectively, can be expressed as

$$\phi_i(r_2) = \phi_{1s}(r_2) = (\gamma_1^3/\pi)^{1/2} \exp(-\gamma_1 r_2) \tag{5}$$

with $\gamma_1 = 1$ and

$$\phi_f(r_1) = \phi_{nlm}(r_1) = N_{nlm} R_{nl}(r_1) Y_{lm}(\theta_1, \phi_1) \tag{6}$$

with $$N_{nlm} = \frac{(2\gamma_n)^{l+1}}{(n+l)!} \left[\frac{\gamma_n (n-l-1)!}{n(n+l)!}\right]^{1/2} \tag{7}$$

$$R_{nl}(r_1) = r_1^l \exp(-\gamma_n r_1) L_{n+l}^{2l+1}(2\gamma_n r_1), \tag{8}$$

where $\gamma_n = \frac{Z}{n}\frac{M}{2}$ ($Z = 1$ for protonium).

In view of eq. (3), the scattering amplitude g_{if}^{FBA} may be written as

$$g_{if}^{\mathrm{FBA}} = -\frac{2M}{2\pi(2M+1)}(I+J), \tag{9}$$

where $$I = -\int \exp[i(\alpha.r_2 - \beta.r_1)] \times \phi_f^*(r_1)(1/r_2)\phi_i(r_2)\, dr_1 dr_2, \tag{10}$$

$$J = \int \exp[i(\alpha.r_2 - \beta.r_1)] \times \phi_f^*(r_1)\left(1/|r_1 - r_2|\right)\phi_i(r_2)\, dr_1 dr_2. \tag{11}$$

Let us first concentrate on the integral J whose evaluation is rather difficult because of the existence of the interaction $(1/|r_1 - r_2|)$. Using the Fourier transform technique and the following integral representation due to Feynman [13]

$$\frac{1}{ab} = \int_0^1 dx [ax + b(1-x)]^{-2}, \tag{12}$$

the integral J becomes

$$J = -A_1 \frac{\partial}{\partial \gamma_1} \int_0^1 dx \int dP \frac{\exp[i(P-\beta).r_1]}{\left[\{P - \alpha(1-x)\}^2 + \mu^2\right]^2} \times R_{nl}(r_1) Y_{lm}^*(\theta_1, \phi_1)\, dr_1, \tag{13}$$

where $A_1 = (2\gamma_1^{3/2}/\pi^{3/2}) N_{nlm}$ and $\mu^2 = (1-x)(\gamma_1^2 + \alpha^2 x)$.

Next, the integration over P is performed and we are left with

$$J = -A_1 \pi^2 \frac{\partial}{\partial \gamma_1} \int_0^1 dx\, \mu^{-1} G, \tag{14}$$

where $$G = \int \exp[i\delta.r_1 - \mu r_1] R_{nl}(r_1) Y_{lm}^*(\theta_1, \phi_1)\, dr_1 \tag{15}$$

with $\delta = \alpha(1-x) - \beta$. Then following Roy *et al* [14], the above integral can be written as

$$G = -A_2 (2\delta)^l Y_{lm}^*(\hat{\delta}) \left[\frac{\partial \Delta}{\partial \mu} C_{n-l-1}^{l+1}(\eta) + 2(l+1)\Delta \frac{\partial \eta}{\partial \mu} C_{n-l-2}^{l+2}(\eta) \right], \quad (16)$$

where $A_2 = 4\pi i^l (n+l)!\, l!$,

$$\eta^2 = \frac{\left[\delta^2 + \mu^2 - \gamma_n^2\right]^2}{\left[\delta^2 + (\mu+\gamma_n)^2\right]\left[\delta^2 + (\gamma_n - \mu)^2\right]},$$

$$\Delta^2 = \left[\delta^2 + (\gamma_n - \mu)^2\right]^{n-l-1} \left[\delta^2 + (\mu+\gamma_n)^2\right]^{-(n+l+1)},$$

and $C_{n-l-1}^{l+1}(\eta)$ and $C_{n-l-2}^{l+2}(\eta)$ are the Gegenbauer polynomials.

In view of eqs. (14) and (16), the final form of J is given by

$$J = A_1 A_2 \pi^2 \frac{\partial}{\partial \gamma_1} \int_0^1 dx\, \mu^{-1} (2\delta)^l Y_{lm}^*(\hat{\delta}) \times \left[\frac{\partial \Delta}{\partial \mu} C_{n-l-1}^{l+1}(\eta) + 2(l+1)\Delta \frac{\partial \eta}{\partial \mu} C_{n-l-2}^{l+2}(\eta) \right]. \quad (17)$$

Now, we move on to the integral I given by eq. (10). After r_2 integration the integral I reduces to the following form

$$I = -4\gamma_1^{3/2} \pi^{1/2} (\alpha^2 + \gamma_1^2)^{-1} N_{nlm} \times \int \exp[-i\beta.r_1] R_{nl}(r_1) Y_{lm}^*(\theta_1, \phi_1) dr_1. \quad (18)$$

The similarity in form between the above integral and G in eq. (15) suggests the use of the result in eq. (16) with δ replaced by β and μ tending to zero. Finally, the integral I thus becomes

$$I = \frac{16 i^l (\gamma_1 \pi)^{3/2} l!(n+l)! 2n\gamma_n (2\beta)^l}{(\alpha^2 + \gamma_1^2)(\beta^2 + \gamma_n^2)^{l+2}} \times N_{nlm} Y_{lm}^*(\hat{\beta}') C_{n-l-1}^{l+1}(\eta') \quad (19)$$

with $\eta' = (\beta^2 - \gamma_n^2)/(\beta^2 + \gamma_n^2)$ and $\beta' = -\beta$. The above expression of the integral I is well known.

Now, the Gegenbauer polynomials can be expressed in terms of hypergeometric series [15] and in view of that, I and J can be recast into the following forms :

$$I = \frac{16 S i^l (\gamma_1 \pi)^{3/2} l!\, 2^{(l+1)} (2\beta)^l 2n\gamma_n}{(2l+1)!(\alpha^2 + \gamma_1^2)(\beta^2 + \gamma_n^2)^{l+2}} \times Y_{lm}^*(\hat{\beta}')\ {}_2F_1(a,b,c;(1-\eta')/2), \quad (20)$$

$$J = -\frac{8 S i^l (\gamma_1 \pi)^{3/2} l! 2^{(l+1)}}{(2l+1)!} \frac{\partial}{\partial \gamma_1} \int_0^1 dx\, \mu^{-1} (2\delta)^l Y_{lm}^*(\hat{\delta}) \times \left[\frac{\partial \Delta}{\partial \mu}\ {}_2F_1(a,b,c;(1-\eta)/2) + \frac{[n^2 - (l+1)^2]}{2l+3} \Delta \times \frac{\partial \eta}{\partial \mu}\ {}_2F_1(a+1, b+1, c+1; (1-\eta)/2) \right] \quad (21)$$

with $S = \gamma_n^{l+3/2} n^l \left[\prod_{r=0}^{l} \left(1 - \frac{r^2}{n^2}\right) \right]^{1/2}$,

$a = n + l + 1$,

$b = -n + l + 1$,

$c = l + 3/2$.

The one-dimensional integration in eq. (21) can be easily performed numerically.

Distorted wave approximation :

In distorted wave approximation, the interaction potential V is modified with the introduction of one distorting potential U. According to Bassel and Gerjuoy [12], the transition amplitude using eq. (2), may be written as

$$g_{if}^{\mathrm{DWA}} = -\frac{2M}{2\pi(2M+1)} \int \exp[i(\alpha.r_2 - \beta.r_1)] \times \phi_f^*(r_1)(V-U)\phi_i(r_2) dr_1 dr_2, \quad (22)$$

where [in view of eq. (3)]

$$V - U = \left(\frac{1}{|r_1 - r_2|} - \frac{1}{r_2} \right) - \left(\frac{1}{r_1 - r_2} + 1 \right) \times \exp[-2|r_1 - r_2|]. \quad (23)$$

In view of eq. (9), the amplitude can be written as

$$g_{if}^{\mathrm{DWA}} = -\frac{2M}{2\pi(2M+1)} (I + J + K), \quad (24)$$

where I and J are given by eqs. (10) and (11) and the third term which represents the correction to the Born amplitude may be written as

$$K = \left(-1 + \frac{\partial}{\partial y} \right) \int \exp[i(\alpha.r_2 - \beta.r_1)] \phi_f^*(r_1) \phi_i(r_2) \times \frac{\exp[-y|r_1 - r_2|]}{|r_1 - r_2|} dr_1 dr_2 \quad (25)$$

with $y = 2$.

The integrand of the above integral is equal to that of J in eq. (11) multiplied by the exponential term $[\exp(-y|r_1 - r_2|)]$ and a similar procedure can be adopted for its evaluation.

3. Results and discussion

The calculated cross sections for $p\bar{p}$ formation in arbitrary excited state (nlm) in $\bar{p} - H(1s)$ collision using first Born approximation (FBA) and distorted wave approximation (DWA) are presented in Figures 1–6 and Table 1.

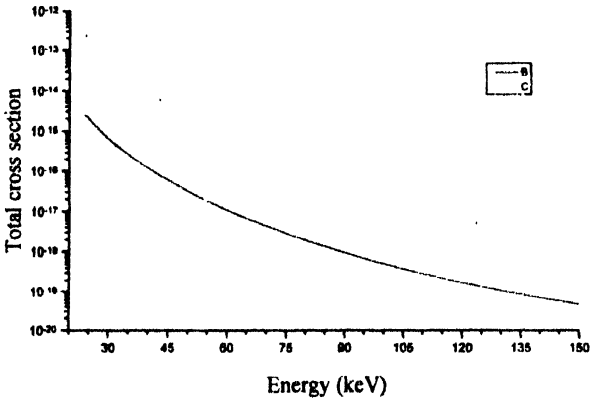

Figure 1. Total cross sections (πa_0^2) for $p\bar{p}$ formation in $n = 5$ state in $\bar{p} - H(1s)$ collision using FBA (B) and DWA (C).

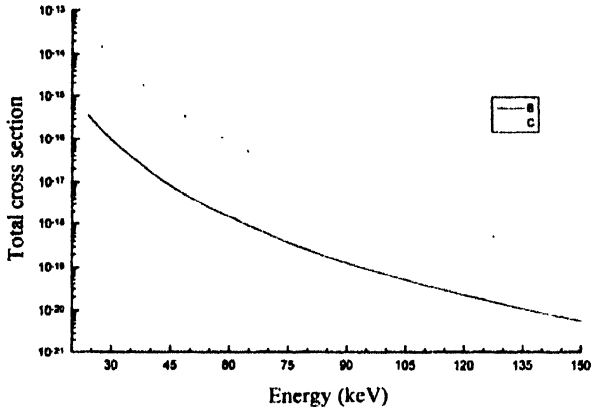

Figure 2. Total cross sections (πa_0^2) for $p\bar{p}$ formation in $n = 10$ state in $\bar{p} - H(1s)$ collision using FBA (B) and DWA (C).

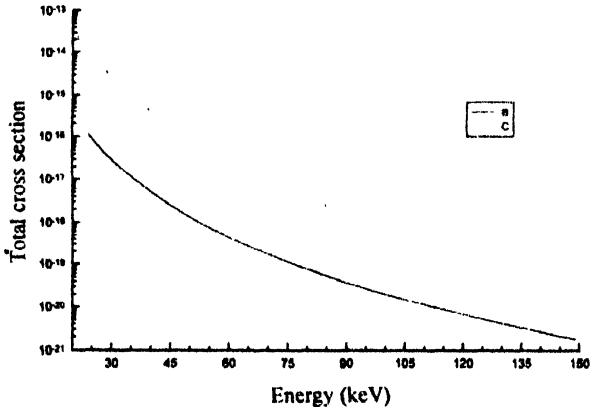

Figure 3. Total cross sections (πa_0^2) for $p\bar{p}$ formation in $n = 15$ state in $\bar{p} - H(1s)$ collision using FBA (B) and DWA (C).

All the numerical results have been obtained from a general computer program by supplying, as inputs, the principal quantum number n and the incident energy E only. There is a provision for cross section evaluation for all admissible values of l and m corresponding to a particular value of n. However, the contributions from different values of m are summed up while the variation of the FBA and the DWA cross sections with l for different values of n and E

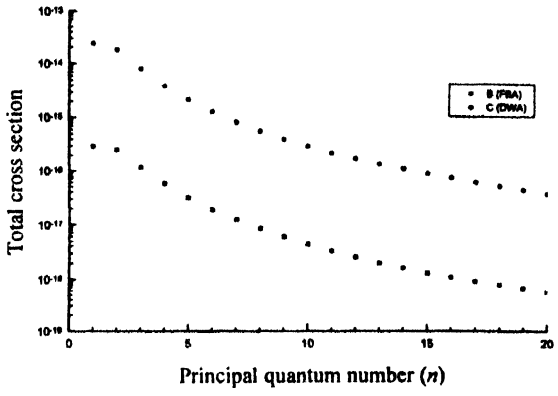

Figure 4. Variation of FBA (B) and DWA (C) cross sections (πa_0^2) with $n(1 \le n \le 20)$ at $E = 50$ keV.

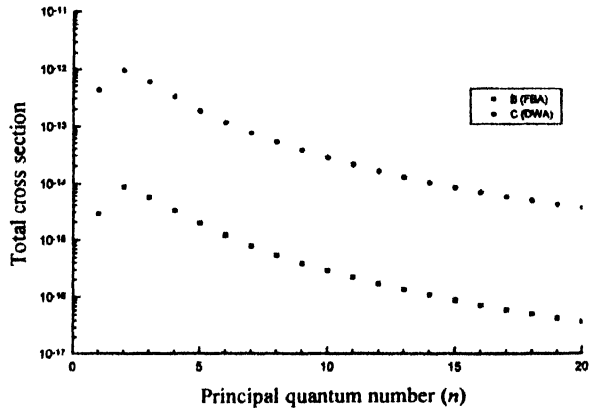

Figure 5. Variation of FBA (B) and DWA (C) cross sections (πa_0^2) with $n(1 \le n \le 20)$ at $E = 25$ keV

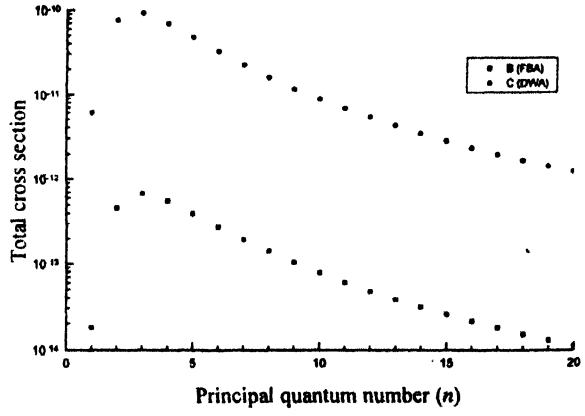

Figure 6. Variation of FBA (B) and DWA (C) cross sections (πa_0^2) with $n(1 \le n \le 20)$ at $E = 10$ keV.

are given in Table 1. It is noted from Table 1 that the cross section values increase intially and then after a certain value of l, decrease sharply. It has been observed that this certain

Table 1. FBA and DWA cross sections (in units of πa_0^2) for $p\bar{p}$ formation in different angular momentum states.

E (keV)	l	FBA $n = 5$	DWA $n = 5$	FBA $n = 10$	DWA $n = 10$	FBA $n = 20$	DWA $n = 20$
	0	1.055 (–16)	4.256 (–14)	1 376 (–17)	5.877 (–15)	1.737 (–18)	7.531 (–16)
	1	1.118 (–15)	1 096 (–13)	1.580 (–16)	1.593 (–14)	2.038 (–17)	2.068 (–15)
	2	6.023 (–16)	3.166 (–14)	9.797 (–17)	5 298 (–15)	1.305 (–17)	7.105 (–16)
	3	7.864 (–17)	2.653 (–15)	1.822 (–17)	6 335 (–16)	2.609 (–18)	9.134 (–17)
	4	2.789 (–18)	6 611 (–17)	1.509 (–18)	3.692 (–17)	2.470 (–19)	6 088 (–18)
25	5			6.533 (–20)	1.191 (–18)	1.336 (–20)	2 456 (–19)
	6			1.580 (–21)	2.237 (–20)	4.594 (–22)	6.560 (–21)
	7			2 143 (–23)	2.433 (–22)	1 073 (–23)	1.228 (–22)
	8			1 523 (–25)	1.419 (–24)	7.822 (–30)	7.354 (–29)
	9			4.399 (–28)	3.437 (–27)	6.646 (–33)	5.236 (–32)
	0	9.426 (–18)	1.069 (–15)	1.242 (–18)	1.426 (–16)	1.574 (–19)	1 811 (–17)
	1	1.797 (–17)	9.278 (–16)	2.450 (–18)	1 282 (–16)	3.130 (–19)	1.642 (–17)
	2	3 818 (–18)	1 178 (–16)	5.948 (–19)	1 863 (–17)	7 836 (–20)	2 464 (–18)
	3	2.239 (–19)	4.632 (–18)	4.957 (–20)	1.043 (–18)	7.014 (–21)	1.481 (–19)
	4	3.736 (–21)	5.565 (–20)	1.929 (–21)	2.924 (–20)	3.119 (–22)	4 748 (–21)
50	5			4.011 (–23)	4.608 (–22)	8 105 (–24)	9.353 (–23)
	6			4.715 (–25)	4.263 (–24)	1 355 (–25)	1.230 (–24)
	7			3 134 (–27)	2.296 (–26)	1.549 (–27)	1 140 (–26)
	8			1.096 (–29)	6.664 (–29)	5.561 (–34)	3.397 (–33)
	9			1.564 (–32)	8.049 (–32)	2 333 (–37)	1 206 (–36)

value of l depends on both n and E. However, it may be mentioned that contributions from the substates having values of l up to 7 have been considered in representing the *total cross section* (in units of πa_0^2) which is the sum of the contributions of all degenerate states with various admissible values of l and m corresponding to a specific n value. From Table 1, it is noted that in case of FBA results corresponding to $E = 25$ keV, contributions from $l = 0$ and $l = 1$ states to the total cross sections are 64.15% for $n = 5$, 59.32% for $n = 10$ and 58.15% for $n = 20$ while in the case of DWA the corresponding figures are 81.57%, 78.5% and 77.7%, respectively. As energy increases to 50 keV, in case of FBA the corresponding figures are 87.13%, 85.1% and 84.59% while they are 94.22%, 93.22% and 92.96% in case of DWA. Thus, in both the approximations, maximum contributions to total cross sections come from $l = 0$ and $l = 1$ states as expected.

In Figures 1–3, the FBA and DWA cross sections have been plotted against E ranging from 25 keV to 150 keV corresponding to $n = 5$, $n = 10$ and $n = 15$, respectively. In Figure 1, the curve corresponding to FBA starts from a maximum and then falls gradually with the increase in E. The nature of the curve corresponding to DWA in this figure is the same as the nature of the curve for FBA but it is above the corresponding FBA curve throughout the energy range considered. The qualitative nature of the curves corresponding to FBA and DWA in Figures 2 and 3, is more or less similar to the nature of the corresponding curves in Figure 1. However, as n increases both the FBA and DWA cross section values become smaller for the protonium wave function has relatively more oscillations then and thereby the integral leading to cross section becomes smaller. A comparative study between the two sets of curves shows that DWA cross sections are, on the average, two order of magnitude larger than the corresponding FBA cross sections throughout the considered energy range which demonstrates the significant improvement of the cross section results over the corresponding FBA ones caused due to the consideration of the non-orthogonality effect. However, it has been observed that asymptotically DWA cross sections have the tendency to approach the corresponding FBA values.

In Figures 4–6, the variations of the FBA and the DWA cross sections with principal quantum number n ($1 \leq n \leq 20$) have been displayed for 50 keV, 25 keV and 10 keV incident energies, respectively. It is noted from these figures that as the incident energy decreases, maximum contributions come from higher excited states irrespective of the approximation considered. In case of $E = 10$ keV maximum contribution comes from $n = 3$ while it is from $n = 2$ and $n = 1$ for $E = 25$ keV and $E = 50$ keV, respectively. Thus, it is evident

from Figures 4–6 and the results discussed earlier, that the cross sections have a tendency to become larger when the incident energy approaches lower values as well as the states of $p\bar{p}$ are of moderately high excitation. This may be explained as follows :

The matrix element for the protonium formation process [eq. (1)] will be significant when the binding energy of the excited $p\bar{p}$ is of the order of the hydrogen atom binding energy and the momenta in the initial and the final channels are small. Both these conditions will be fulfilled simultaneously when the $p\bar{p}$ atom is formed in moderately high excited state and the incident energy is rather small. For very high excited state however, the final bound-state wave function has many oscillations and as a result, the integral leading to cross section is extremely small.

4. Conclusion

We present a full quantum mechanical approach for the evaluation of the FBA transtion amplitude for protonium formation in an arbitrary excited state without any restriction on the quantum numbers n, l and m. In this approach, the amplitudes have been reduced to one-dimensional integrals which are amenable to easy numerical evaluations. Application of this technique to the DWA incorporating the effect of non-orthogonality has also been shown. Two interesting features have been noticed during the analysis of the presented results. The orthogonality correction provides considerable improvement over the FBA results and the calculated cross sections in both the approximations have a tendency to become appreciable when projectile energy is low as well as the $p\bar{p}$ is formed in moderately high excited states.

It is well known that the FBA and DWA are essentially high-energy approximations. However, we feel that due to the inherent complications of the problem, a full quantum mechanical approach using such approximations is of interest and is helpful to get a qualitative understanding of the main features of the formation process. Moreover, such study is also helpful in providing a guideline for further activities in this field.

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